2,2,3,3,4,4,5,5,6,7,7,7-Dodecafluoro-6-(trifluoromethyl)heptanoic acid
15166-06-0 | DTXSID50562865

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.12

Global applicability domain: Inside

Local applicability domain index: 3.93e-01

Confidence level: 3.89e-01

Nearest Neighbors from the Training Set

Image not found
1,1,2,2-Tetrahydroperfluoro-1-decanol
Measured: 5.58
Predicted: 5.05

Image not found
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol
Measured: 4.54
Predicted: 4.45

Image not found
Perflenapent
Measured: 4.40
Predicted: 4.23

Image not found
1-Dodecyl-2,4-dimethylpyridin-1-ium iodide
Measured: 1.41
Predicted: 4.25

Image not found
Midaflur
Measured: 3.35
Predicted: 3.49